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Renormalized series calculations of the spectra of anharmonic oscillators

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Abstract : The energy levels of the Schrödinger equation for many polynomial forms of potentials have been calculated, using renormalized hypervirial perturbation (renormalized series) for various values of perturbation parameters and state numbers n Results of good accuracy are produced for various eigenstates and over a wide ranges values of perturbation parameters.

Keywords : Schrödinger equation, renormalized series, different forms of potentials.

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1. A symmetric perturbation

The study of one-dimensional anharmonic oscillators has evoked much interest because of its varied application in field theory [1] and molecular physics [2]. A general survey of the various applications may be found in the literature [3,4].

In the literature there are several papers [5–7] investigated the general properties, approximation schemes, and numerical calculations for the one-dimensional oscillator.

Doubly anharmonic systems of the type $\lambda_2 x^2 + \lambda_4 x^4 + \lambda_6 x^6$ has been studied analytically [8–11] and numerically [12,13]. Also this type of the potential, can serve as a useful model in certain situations of physical interest. It has been used in calculations of the vibrational spectra of molecules [14] and in a description of the behaviour of a ^{3}He–^{4}He mixture and so-called metamagnets near the tricritical point [15]. Some anharmonic oscillators with more complicate potentials have also been investigated recently [16,17,18].

The Schrödinger equation for the anharmonic oscillator with polynomial potentials can be expressed as

$$\frac{d^2}{dx^2} + V(x)\ \Psi(x) = E\Psi(x), \tag{1.1}$$

where

$$V(x) = v_2 x^2 + \sum_{2I=2}^{14} \lambda^2 v_{2I} x^{2I}, \qquad \lambda = 1. \tag{1.2}$$

The methods of calculations start from the recurrence relations which derived from the hypervirial and Hellmann-Feynman theorems and have been used by the author [16] in the form

$$2E(N+1)\langle x^N\rangle = \sum v_I(2N+2+I)\langle x^{N+I}\rangle - \frac{N}{2}\left(N^2-1\right)\langle x^{N-2}\rangle. \tag{1.3}$$

The next step, assuming that the energy E and the expectation values $\langle x^N\rangle$ can be expanded in power series of the perturbation parameter λ as

$$E = \sum E(L)\lambda^L, \tag{1.4}$$

$$\langle x^N\rangle = \sum F(N,M)\lambda^M. \tag{1.5}$$

In order to improve the convergence properties of the perturbation series we used a rearrangement of terms in the potential given by (1.2). To illustrate this technique it is necessary to write the potential in renormalized form

$$V_r(x) = [\mu - \lambda K]x^2 + \sum_{2I=4}^{14} \lambda^2 v_{2I} x^{2I}, \tag{1.6}$$

where

$$\mu = v_2 + \lambda K. \tag{1.7}$$

The use of the renormalization parameter K is helpful in improving the convergence. If we use the perturbation expansions (1.4) and (1.5) in the hypervirial relation given by (1.3), we obtain the following recurrence relations corresponding to the potential (1.6) as follows :

$$(2N+2)\sum_{0}^{M} E(L)F(N,M-L) = -\frac{N}{2}\left[N^2-1\right]F(N-2,M),$$

$$(2N+4)\left[\mu F(N+2,M) - KF(N+2,M-1)\right] + \sum_{2I=4}^{14} v_{2I}$$

$$\times\left(2N+2+2I\right)F(N+2I,M-2). \tag{1.8}$$

Applying the Hellmann-Feynman theorem in the form

$$\frac{\partial E}{\partial \lambda} = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle = \left\langle \frac{\partial V}{\partial \lambda} \right\rangle \tag{1.9}$$

to the renormalized potential (1.6), we obtain the following, a recurrence relation

$$(M+1)\,E(M+1) = 2\sum_{2I=4}^{14} v_{2I}F(2I, M-1) - KF(2, M). \tag{1.10}$$

The unperturbed energy corresponding to the potential given by eq. (1.6) can be expressed as

$$E = (2n + 1)\sqrt{\mu} \qquad (n = 0, 1, 2, \ldots). \tag{1.11}$$

The recurrence relations (1.8) and (1.10) suffice to compute the coefficients of energy $E(M)$ and $F(N,M)$ and this procedure allows us to calculate the expectation values of powers $\langle x^N \rangle$ without the explicit use of the wave functions. The input for our calculations are the renormalization parameter K and the state number n. The values of $\mu = 1 + \lambda K$, $E(0) = (2n + 1)\sqrt{\mu}$, are worked out by the program. The renormalized series approach seems to give results of good accuracy, whereas at $K = 0$ the perturbation series diverge and not give satisfactory numerical results.

In the present work, we applied the renormalized series method to calculate the energy eigenvalues for the polynomial potentials (1.2) for different values of the coefficients ($0 \le v_{2I} \le 10^6$; $2I = 2$ to 14), λ and state numbers $0 \le n \le 100$, the results listed in Table 1 and compared them with those produced by power series method. The renormalized series

Table 1. Energy eigenvalues of $H = P^2 + x^2 + \sum_{2I=4}^{14} \lambda^2 V_{2I} x^{2I}$ at $\lambda = 1$, the results with all digits are the finite difference calculations, and those with an underline are renormalized series calculations.

n	V_4	V_6	V_8	V_{10}	V_{12}	V_4	V_6	V_8	V_{10}	V_{12}	V_{14}
	10^6	10^6	10^6	10^6	10^6	10^6	10^6	10^6	10^6	10^6	10^6
0		106.57412561						106.57412 58			
5		2151.33655689						2151.33665 22			
10		5125.53440164						5125.53586 73			
15		8664.23393170						8664.24204 35			
20		12644.27280299						12644.30068 8			
25		16997.58956646						16997.66253 92			
50		43170.791819 9						43172.214539			
100		111813.201999						111838.377699			
	10^5	10^5	10^5	10^5	10^5	10^5	10^5	10^5	10^5	10^5	10^5
0		49.7643538 1						49.764357 2			
5		1013.7352697 0						1013.737019 2			
10		2434.8643973 1						2434.889401 4			

Table 1. (*Contd.*)

n	V_4	V_6	V_8	V_{10}	V_{12}	V_4	V_6	V_8	V_{10}	V_{12}	V_{14}
	10^6	10^6	10^6	10^6	10^6	10^6	10^6	10^6	10^6	10^6	10^6
15		4144.93232638						4145.06176335			
20		6087.67655702						6088.09487004			
25		8232.25107936						8233.28426020			
50		21447.43044525						21463.13092220			
	10^4	10^4	10^4	10^4	10^4	10^4	10^4	10^4	10^4	10^4	10^4
0		23.41049229						23.41056433			
5		486.44528420						486.47173733			
10		1189.61956350						1189.94072776			
15		2056.77343421						2058.20863210			
	10^4	10^4	10^2	10^2	10^2	10^4	10^4	10^4	10^2	10^2	10^2
0		23.364712466						23.405705757			
5		481.910743335						485.646343434			
10		1166.408593332						1184.085345			
15		1994.86196455						2039.253005			
	10^3	10^3	10^3	10^3	10^3	10^3	10^3	10^3	10^3	10^3	10^3
0		11.209689233						11.210695224			
5		243.06643573						243.32820348			
10		616.98561922						619.28474307			

method works extremely well for the potential (1.2), but for higher values of the coefficients v_{2l} and state numbers n, the power series gives a better accuracy than the renormalized series. Also we did some checks for some of our results by applied the finite difference method and the agreement is good.

Also we extend the numerical calculation to the three-dimensional case

$$V(r) = r^2 + l(l+1)r^{-2} + v_4\lambda^2 r^4 + v_6\lambda^2 r^6 + v_8\lambda^2 r^8, \quad \lambda = 1. \tag{1.12}$$

The main difference between (1.2) and (1.12) lies in the angular momentum term $l(l+1)r^{-2}$. Using hypervirial and Hellmann-Feynman theorems as used for one dimensional case we obtain the following recurrence relation

$$(2N+2)\sum_{0}^{M} E(L)F(N,M-L) = \left[2Nl(l+1) - \frac{N}{2}\left(N^2-1\right)\right]F(N-2,M)$$

$$+ (2N+4)\left[\mu F(N+2,M) - KF(N+2,M-1)\right] + v_4(2N+6)F(N+4,M-2)$$
$$+ v_6(2N+8)F(N+6,M-2) + v_8(2N+10)F(N+8,M-2) \quad (1.13)$$

$$(M+1)E(M+1) = 2v_4 F(4,M-1) + 2v_6 F(6,M-1) + 2v_8 F(8,M-1)$$
$$- KF(2,M). \quad (1.14)$$

The unperturbed energy corresponding to the potential given by eq. (1.12) can be expressed as

$$E = (4n_r + 2l + 3)\sqrt{\mu}, \quad (1.15)$$

where l and n_r are called the angular momentum and radial quantum number respectively. We listed our results for potential (1.12) in Table 2, for different values of quantum numbers (n_r and l) and over wide range values of (v_4, v_6, v_8), we compare our results with those produced by power series.

Table 2. Energy eigenvalues of $V(r) = r^2 + l(l+1)\,r^{-2} + v_4\lambda^{-4} + v_6\lambda^{-6} + v_8\lambda^{-8}$ at $\lambda = 1$; the results with all digits are the power series calculations, and those with an underline are renormalized series calculations.

n_r	l	v_4	v_6	v_8	$E_{n_r l}$	M	K
1	1	10^2	10^2	10^2	92.1401906095743	104	2500
1	1	10^2	10^3	10^2	128.1372957828276	95	3200
1	1	10^3	10^3	10^3	178.6145677213552	78	5200
10	10	10^3	10^2	10^2	2294.5118412094050	142	8200
10	10	10^3	10^3	10^2	2694.1977914977313	173	12000
10	10	10^3	10^3	10^3	2921.2720339536001	180	17000
0	10	10^2	10^2	10^2	305.3383757274058	207	6000
10	0	10^2	10^2	10^2	948.2392243975153	197	6000
0	100	10^2	0	0	4169.2014223521495	218	10000
0	100	0	10^2	0	5711.3955626897358	215	16000
0	20	10^2	10^2	10^2	752.1806808813684	217	6000
0	15	10^2	10^2	10^2	512.0402209085576	197	7000
5	5	10	10	10	359.7759985051161	201	4000
5	5	10^2	10^2	10^2	621.3869926514746	180	5000
5	5	10^3	10^3	10^3	1131.1815294255389	111	8000
0	5	10^3	10^3	10^3	266.8175342046574	119	7000
5	0	10^3	10^3	10^3	685.3622486445382	105	7000

Table 2. (*Contd.*)

n_r	l	v_4	v_6	v_8	$E_{n_r,l}$	M	K
0	0	10^3	10^3	10^3	40.52847439 56459	117	7000
15	15	10^3	10^3	10^3	5219.91479085 99012	130	18000
15	15	10^3	0	0	3597.62568150 90510	111	80000
25	25	10^4	10^4	10^4	19776.98271029 75313	83	38000
25	25	10^4	10^4	0	18280.61956438 53477	89	38000
0	25	10^4	10^4	10^4	3632.44626278 86319	150	38000
50	50	10^5	10^5	10^5	99855.43749900 1	200	10^6
50	50	10^5	10^5	0	94385.66114598	216	10^6
50	50	10^5	0	0	80632.70103278 6	220	10^6
0	50	10^5	10^5	10^5	18302.85844077 525	212	400000
50	0	10^5	10^5	10^5	57223.38560000 1	214	400000
0	0	10^4	10^4	10^4	178.77485248129 98	53	30000

We have discovered that the renormalized series method will work a better for the perturbed potentials (1.2), if we taking different power of λ_{-1}^{J1}; $\lambda_{-2}^{J2} J1, J2 = 1, 2, 3, 4,$ instead of λ, we took two types of potentials as the examples to show the applicability of this technique to improve the convergence of the perturbation series. If we applied the techniques λ_{-1}^{J1}; and λ_{-2}^{J2} to the potential (1.2), we obtain the following forms corresponding to these examples

$$V(x) = x^2 + \lambda_{-1}^{J1} v_4 x^4 + \lambda_{-2}^{J2} v_6 x^6, \tag{1.16}$$

$$V(x) = x^2 + \lambda_{-1}^{J1} v_4 x^4 + \lambda_{-2}^{J2} v_8 x^8. \tag{1.17}$$

By employing the hypervirial relation (1.3) and using perturbation expansions (1.4) and (1.5) to the potentials (1.16) and (1.17), the following recurrence relations are obtained

$$(2N+2)\sum_{0}^{M} E(L)F(N,M-L) = -\frac{N}{2}\left[N^2-1\right]F(N-2,M)$$

$$+ (2N+4)\left[\mu F(N+2,M) - KF(N+2,M-1)\right] + v_4(2N+6)F(N+4,M-J1)$$

$$+ v_{2m}(2N+2P)F(N+2m,M-J2) \quad m = 3, 4; J1, J2 = 1, 2, 3, 4..., \tag{1.18}$$

where

$$\mu = 1+\lambda_{-1}K; \quad \lambda_{-1} = \lambda^{\frac{1}{J1}}, \quad \lambda_{-2} = \lambda^{\frac{1}{J2}}. \tag{1.19}$$

Applying the Hellmann-Feynman theorem given by eq. (1.9) to potentials (1.16) and (1.17), we obtain a recurrence relation for the energy coefficients in the form

$$(M+1)E(M+1) = J1\, v_4 F(4,M-J1) + J2\, v_{2m} F(2m,M-J2) - KF(2,M). \tag{1.20}$$

The energy eigenvalues for the double perturbation anharmonic oscillator defined by the potentials (1.16) and (1.17) have been calculated by applied the technique of various power of λ^{J1} and λ^{J2} together with different values of the renormalization parameter K. In this technique, we exploit the various power of ($J1$ and $J2$) together with values of the renormalization parameter K to achieve results with the best accuracy. It is interesting to apply λ^{J1} and λ^{J2} technique to produce perturbation series with a better convergence than the original perturbation series with ($J1 = J2 = 1$), the numerical example to clarified this situation is that, if we look to Table 3, at $\lambda_1 = \lambda_2 = 10$; $J1 = J2 = 1$; $\nu_4 = \nu_6 = 1$, the eigenvalue has poor accuracy and equal to 3.1, but the accuracy improves with another values of parameters $\lambda_1 = \lambda_2 = 10$; $J1 = 2$, $J2 = 4$; $\nu_4 = 10^2$, $\nu_6 = 1$, and the eigenvalue corresponding to this set of

Table 3. Energy eigenvalues of $H = P^2 + x^2 + V_4\,\lambda_1^{J1}x^4 + V_{2m}\,\lambda_2^{J2}x^{2m}$, First line; power series calculation, other lines; renormalized series calculations.

$2m$	$J1$	$J2$	λ_1	λ_2	V_4	V_{2m}	E_0	M	K
							1 151518875960		
6	4	4	0.1	0.1	1	1	1.151518875	161	60
	1	1	0.1	0.1	1	1	1.151518	71	220
	1	4	0 1	0.1	10^{-3}	1	1.151518875	184	70
							1.614894082031		
	4	4	1	1	1	1	1 61489408	156	100
	1	1	1	1	1	1	1.6148	189	250
	1	4	1	1	1	1	1.614894082	154	90
	4	1	1	1	1	1	1.614894	101	100
	3	1	1	1	1	1	1.614894	106	100
	1	3	1	1	1	1	1.614894082	169	90
							2 794087177819		
	4	4	10	10	1	1	2.79408717	136	180
	1	1	10	10	1	1	3.1	55	120
	1	1	1	1	10	10	2 79408	57	180
	2	4	10	10	10^2	1	2 79408717	151	180
							5.425470091197		
	4	4	1×10^2	1×10^2	1	1	5 4254701	119	350
	1	1	1	1	10^2	10^2	5.42547	81	920
	2	4	10^2	10^2	10^4	10^2	5 42547009	109	280
							6 706460210563		
	1	4	2×10^2	2×10^2	1	1	6.7064602	133	350

Table 3. (*Contd.*)

$2m$	$J1$	$J2$	λ_1	λ_2	V_4	V_{2m}	E_0	M	K
	6	6	2×10^2	2×10^2	1	1	6.706460	131	900
	2	2	1	1	2×10^2	2×10^2	6.706460	132	2000
	2	4	2×10^2	2×10^2	4×10^4	1	6.70646021	104	340
							11.11494230370		
	4	4	10^3	10^3	1	1	11.11494	85	800
	4	4	1	1	10^3	10^3	11.1149423	165	6000
	2	4	10^3	10^3	10^6	1	11.11494230	81	440
							23.36424510195		
	4	4	10^4	10^4	1	1	23.3642	51	1200
	4	4	1	1	10^4	10^4	23.36424510	112	15500
	2	2	10^4	10^4	10^8	10^8	23.364245101	59	750
	1	1	10^4	10^4	10^{12}	10^{12}	23.3642451	55	780
8							1.2022691851		
	6	6	0.1	0 1	1	1	1.20226	161	140
	3	3	0.1	0 1	10^{-3}	10^{-3}	1.202	136	210
	4	4	0.1	0.1	1	1	1.20226	116	120
							1 6451639251		
	6	6	1	1	1	1	1.6451	100	175
	3	3	1	1	1	1	1.645	111	300
							2.7125103247		
	6	6	10	10	1	1	2.7125	122	390
	3	3	10	10	10^3	10^3	2 712	116	580
							5.1824766428		
	6	6	10^2	10^2	1	1	5.18247	123	690
	6	6	1	1	10^2	10^2	5.182476	192	2000
	3	3	10^2	10^2	10^6	10^6	5.182	116	880
							10.738633995		
	6	6	10^3	10^3	1	1	10.73	69	990
	6	6	1	1	10^3	10^3	10.738633	182	7500
	3	3	10^3	10^3	10^9	10^9	10.7386339	125	1400

Table 3. (*Contd.*)

$2m$	$J1$	$J2$	λ_1	λ_2	V_4	V_{2m}	E_0	M	K
	2	2	10^3	10^3	10^6	10^6	10.7386339	79	480
							22.909444802		
	6	6	1	1	10^4	10^4	22.9094448	184	23000
	3	3	10^4	10^4	10^{12}	10^{12}	22.9094448	89	2300
	2	2	10^4	10^4	10^8	10^8	22.909444802	59	700

parameters is 2.79408717, it is clear for this example how this technique can be used to give perturbation series with a better convergence, and this picture can be generalized to other eigenvalues reported in Table 3. The results are compared with those calculated by power series. We did some checks for our results by applying the finite difference method [16] and the agreement is good.

On the other hand, the same technique has been used by the author [16] for single perturbation such as λx^6 and λx^8 and succeeded to improve the convergence of the perturbation series.

2. An asymmetric perturbation

The problem of the anharmonic oscillator with potential

$$V(x) = x^2 + \lambda_3 x^3 + \lambda_4 x^4 + \lambda_5 x^5, \tag{2.1}$$

has been treated by many workers. For example for the case $\lambda_4 = \lambda_5 = 0$ has been treated by Drummond [19,20] and Witwit [21]. On the other hand, the problem which consists of equally weighted cubic and quartic has been studied by the workers [22,23], also the same problem with mixed weighted is treated by the author [24].

The potential (2.1) can be rewritten in terms of the single perturbation parameter λ_3 as

$$V(x) = x^2 + \lambda_3 x^3 + \alpha\lambda_3 x^4 + \beta\lambda_3 x^5 \tag{2.2}$$

with parameters α and β replaced by

$$\alpha = \lambda_4/\lambda_3, \quad \beta = \lambda_5/\lambda_3 \tag{2.3}$$

in this way, we can avoid the use of three-parameter hypervirial relations.

The energy perturbation series is expected to be divergent, so we start by introducing a renormalization parameter K, and write the potentials as given by eq. (2.2) in the renormalized form

$$V^r(x) = \mu x^2 + \left[V(x) - \lambda_3 K x^2\right]; \qquad \mu = 1 + K\lambda_3. \tag{2.4}$$

We shall use the hypervirial relations (1.3) in calculating the perturbation energy series, and inserting the series expansions given by eqs. (1.4) and (1.5) into (1.3) and taking into account the potential coefficients (2.4), we obtain the following recurrence relation after some algebra,

$$(2N+2)\sum_{0}^{M} E(L)F(N,M-L) = -\frac{N}{2}\left[N^2-1\right]F(N-2,M)$$

$$+ (2N+4)\left[\mu AFN+2,M) - KF(N+2,M-1)\right] + [2N+5]F(N+3,M-1)$$

$$+ \alpha[2N+6]F(N+4,M-1) + \beta[2N+7]F(N+5,M-1). \tag{2.5}$$

Applying the Hellmann-Feynman theorem as given by eq. (1.9), to the potential given by eq. (2.4), we obtain a recurrence relation in the form

$$(M+1)E(M+1) = F(3,M) + \alpha F(4,M) + \beta F(5,M) - KF(N+2,M). \tag{2.6}$$

It is clear now that from recurrence relations (2.5) and (2.6) we obtain the full set of $F(N, M)$ and $E(M)$ coefficients starting from the initial condition $F(0,0) = 1$, and the unperturbed energy

$$E(0) = (2n + 1)\sqrt{\mu}. \tag{2.7}$$

One of our main aims in this paper, has been to present a detailed numerical analysis of the applicability of the renormalized series technique to treat potentials with mixed parity. To this end, we have chosen the model potential (2.1), which describes a rather general example of one-dimensional anharmonic oscillators. By choosing different combinations of values for the three perturbation parameters λ_3, λ_4 and λ_5, it has been possible to produce different potential models.

We present, in Table 4, the energy eigenvalues of the anharmonic oscillator with cubic and quartic perturbations as functions of the perturbation parameters λ_3 and λ_4 for several

Table 4. Energy values for $V(x) = x^2 + \lambda_3 x^3 + \lambda_4 x^4 + \lambda_5 x^5$ using renormalized series method for various values of perturbation parameters.

λ_3	λ_4	λ_5	E_0	E_1	E_2	E_3
.005	0.01		1.00735771435469	3.0364272121035	5.0936905158304	7.1781183747758
	0.10		1.06527568399354	3.3068246121398	5.7478648601958	8.3525354306522
	0.25		1.14189585511471	3.6394576000722	6.5008628065024	9.6335679285827
	0.50		1.2418505021099	4.0519194867023	7.3968797843243	11.115126277461
	1.0		1.392349750758	4.648806568188	8.65504054471	13.15679158898
	0.01		1.00576886937146	3.0266191648079	5.0687289016914	7.1322970211534
	0.10		1.06430069945359	3.3021185762077	5.7384921561244	8.3384014650063

Table 4. (*Contd.*)

λ_3	λ_4	λ_5	E_0	E_1	E_2	E_3
	0.25	0	1.14130278361876	3.6370346138601	6.4966102173445	9.6276256007405
	0.50		1.241498138841	4.050647665847	7.394814585105	11.112353642035
	1.0		1.39216252856	4.648199018081	8.65410856255	13.15557289663
0.10	0.01		1.00083993999852	2.9956365665019	4.9884199694797	6.9825277459063
	0.10		1.06131852357717	3.2876938763002	5.7097676470864	8.2951195841333
	0.25		1.1394981346215	3.629662368688	6.4836800715409	9.6095670131943
	0.50		1.240428350985	4.046787613725	7.3885490156833	11.103943609816
	1.0		1.39159475323	4.64635694461	8.65128327808	13.151878736977
λ_3	λ_4	λ_5	E_4	E_5	E_6	E_{10}
0.10	0.01	0	8.9809416863520	10.986259878406	13.000696647723	21.181917013056
	0.10		11.0220409630396	13.874923092764	16.841914325326	29.687195645480
	0.25		12.9605902775959	16.506559598401	20.225956007962	36.557370994951
	0.50		15.1230121295697	19.402013750853	23.910493178110	43.850800904660
	1.0		18.051576650349	23.290478867393	28.827450858074	53.437901941128
0.2	0.10		10.7830824467004	13.579318823101	16.491636086072	29.134893105405
	0.25	0	12.8683623130841	16.396253943586	20.098491208648	36.367873940744
	0.50		15.0813736349748	19.353025144743	23.854564733866	43.769952745110
	1.0		18.033615241176	23.269571687268	28.803768347799	53.404281000603
	1.5		20.178756639207	26.103269277798	32.373260974573	60.301110921738
0.5	0.25		12.181484325	15.580555231	19.1609852443	34.9921935051
	0.50		14.7840149397	19.0040209541	23.4568383591	43.1974580399
	1.0		17.9070810043	23.1224017737	28.6371598917	53.16807765228
	2.0		21.8644314631	28.3337636053	35.18637732384	65.75187282326
	5.0		28.8557548039	37.5166869668	46.70486003031	87.78730233483
	10		35.8773980475	46.7201617192	58.23130116979	109.75871767436
λ_3	λ_4	λ_5	E_0	E_1	E_2	E_3
0.5	0.5	0.0	1.2044787015	3.918226733	7.1820025794	10.8282366831
1.0	1.0	0.0	1.31025753	4.3890214	8.26338075	12.64864211
0.01	0.5	0.01	1.24174017656	4.051282982634	7.3951416045	11.111692971
0.01	1.0	0.1	1.3902715879	4.6362368207	8.6183432096	13.0812998664
0.1	5.0	0.15	2.017589535	7.0102836464	13.460408183	20.8009524294
0.5	100	0.75	4.99925093	17.829637961	34.97294395	54.383608370

Table 4. (*Contd.*)

λ_3	λ_4		E_0		E_2	E_3
1.0	200	1.5	6.262537951	22.3737730463	43.81244461	68.3629555646
2.5	750	3.5	9.67363483	34.6209055415	67.87547409	105.969513229
10	1000	5	10.63821065	38 082626711	74.67507191	116.59470481
100	10^4	100	22.85432404	81.884030839	160.65706017	250.91221542
150	10^4	200	22.84442729	81.85701573	160.61507478	250.85449612
25	1500	15	12.16392103	43.55863859	85.43175664	133.403674069
50	5000	50	18.14834586	65.01343695	127.54397216	199.187111486

λ_3	λ_4	λ_5	E_4	E_5	E_6	E_8
1.0	1.0	0.0	17.443444904	22.58488077	28.030078594	39.712747315
0.01	0.5	0.01	15.1310811164	19 40962283321	23.91689827598	33.5318534194
0.1	1.5	0.15	20.0113532057	25.85114330471	32.01890951229	45.2031917825
0.5	100	0.75	75.8745850211	99 0295735106	123 6364823581	176.622224581
1.5	500	2.5	129.3005431722	168.8321130742	210 8503321336	301.3455663486
10	1000	5	162.79170061	212.581292801	265.5047982398	379 4914777277
100	10^4	100	350.38766119	457.606516923	571.5797406049	817.0682528825
150	10^4	200	350.31361766	457.515472185	571 4710082311	816.9220500538
25	1500	15	186.272675593	243 254602984	303 8242472111	434.2816250151
50	5000	50	278.147648949	363.253599623	453.7200860921	648.5752495548

eigenstates $n = 0, 1, 2, 3, 4, 5, 6, 10$. It appears from our results, that the renormalized series work equally well for small and high values of λ_3 and λ_4. To get the energy eigenvalues of the workers [22–24], it is necessary to multiple their energy values by 2, since they used $-\frac{1}{2}\nabla^2$ in their hamiltonian. The precision of the energies seems good even for excited states, but the previous approaches [22–24] achieved only six figures; our results can thus considered as more accurate.

Also in Table 4, we list the energy for (2.2) for state numbers $n = 0, 1, 2, 3, 4, 5, 6, 8$ for several sets of values of perturbation parameters λ_3, λ_4 and λ_5. We extend our calculation to involve another term of perturbation $\lambda_5 x^5$. To produce result with good accuracy, we must choose the best values of K, and to achieve this choice, we have tested many values of K until we obtained the best convergence .

3. Symmetric double-well potential

The fundamental system of interest to us here is the double-well potential of the form

$$V(x) = -Z^2x^2 + x^{2I}. \tag{3.1}$$

The most studied model system of this kind is the smooth double-well potential of the form with $2l = 4$. A variety of techniques have been used to investigate the eigenvalues and other properties of such a potential [25–29]. Its eigenvalue spectrum has the feature that the lower eigenvalues are closely bunched in pairs if the two wells are sufficiently separated *i.e.* (large values of Z^2).

To calculate energy eigenvalues for the double-well potential, we considered the Schrödinger equation

$$\left(\frac{d^2}{dx^2} - Z^2x^2 + x^{2l}\right)\Psi(x) = E\Psi(x). \tag{3.2}$$

The double-well potential has two minima at $x = \pm x_m$ and one local maximum at $x = 0$. The probability of finding the particle is locally maximal at $x = \pm x_m$. Its low energy levels should involve wave functions which present the maximal probability density at a position close to the minium of the two-well potential. In this case we expand $V(x)$ around the right-hand minimum. Let x_m and $V(x_m)$ be the values of x and $V(x)$, respectively, at the minimum.

It is easy to show that

$$x_m = \left[\frac{Z^2}{l}\right]^{\left[\frac{1}{2l-2}\right]} \tag{3.3}$$

and

$$V(x_m) = -Z^2x_m^2 + x_m^{2l}. \tag{3.4}$$

Let $z = x - x_m$; the Taylor series expansion of $V(x)$ around $z = 0$ can be written as a

$$V(z) = V(x_m) + V'(x_m)z + \frac{1}{2!}V''(x_m)z^2 + \frac{1}{3!}V'''(x_m)z^3 + \sum_{J=4}^{2l} \frac{d^JV(x)}{dx^J}\bigg|_{x=x_m} \frac{z^J}{J!}. \tag{3.5}$$

The central idea of this work is to expand the potential $V(x)$ in a Taylor series about its minimum value, and solve the resulting approximate problem by hypervirial perturbation theory. Physically, as the potential well is very deep (large Z^2 values) the classical turning points for the lowest bound states are very close to the minimum of each well; therefore the particle, even quantum mechanically, can in the main see only the region of the potential near the minima. The lower levels for this potential are almost two-fold degenerate.

The potential $V(z)$ given by (3.5) can be rewritten in terms of the perturbation parameter λ as

$$V(z) = \sum_{J=0}^{2l} \lambda V(J)z^J; \quad \lambda = 1. \tag{3.6}$$

With the coefficients given by eq. (3.5) $\left.\frac{d^J V(x)}{dx^J}\right|_{x=x_n} \frac{1}{J!}$ is replaced by $\lambda V(J)$.

In order to improve the convergence properties of the perturbation series we use a rearrangement of terms in the potential given by (3.6). To illustrate this technique it is necessary to write the potential appearing in eq. (3.6) in renormalized form

$$V(z) = V(x_m) + [\mu - \lambda K]z^2 + \lambda \sum_{I=3}^{2J} V(I) z^J, \tag{3.7}$$

where μ is given the numerical value

$$\mu = 2(I-1)Z^2 + \lambda K. \tag{3.8}$$

If we use the perturbation expansions (1.4) and (1.5) in the hypervirial relation given by eq. (1.3), we obtain the recurrence relation

$$\begin{aligned}(2N+2)\sum_{0}^{M} E(L)F(N,M-L) = & -\frac{N}{2}\left[N^2-1\right]F(N-2,M) \\ & -(2N+4)\left[\mu F(N+2,M) - KF(N+2,M-1)\right] \\ & +\sum_{I=3}^{2J} V(I)(2N+2+I)F(N+I,M-1).\end{aligned} \tag{3.9}$$

Applying the Hellmann-Feynman theorem given by eq. (1.9), we obtain a recurrence relation for the energy coefficients of the form

$$(M+1)E(M+1) = \sum_{J=3}^{2I} V(J)F(J,M) - KF(2,M). \tag{3.10}$$

The unperturbed energy corresponding to the double-well potential can be expressed as

$$E(0) = V(x_m) + (2n+1)\sqrt{\mu} \qquad (n = 0, 1, 2,\ldots). \tag{3.11}$$

From the recurrence relations (3.9) and (3.10) together with the unperturbed energy (3.11) and the initial coefficient value $F(0,0) = 1$, we can calculate sequentially the perturbation series for the $\langle z^N \rangle$ and the energy.

The renormalized series method has been used for calculating the eigenvalues of the double-well potential given by eq. (3.1). Eigenvalues for different values of Z^2, $2I$ and state number n are listed in Table 5.

In Table 5, we list the energy eigenvalue for $2I = 4 - 14$ and for different values of Z^2 and state numbers n. It is clear from the Table 5 that there is agreement between our results and the previous published results of Balsa *et al* [25] and Saavedra and Buendìa [28] up to

decimal places, respectively, at higher values of Z^2; but at lower values of Z^2, it was found that the renormalized series faced greater convergence difficulties.

Table 5. Energy eigenvalues for $H = P^2 - Z^2x^2 + x^{2l}$, for different values of Z^2 and l. We compare our results for the case $2l = 4$. The digits with underlines are the earliest digits to disagree with the values calculated by other workers.

$2l$	Z^2	n	$-E_n$	$2l$	Z^2	n	$-E_n$
4	7	0	8.66678	6	50	0	122.18207663324
	10	0	20 6335$\underline{6}$17929 [25]		50	2	95 59546605
	15	0	50 841387284$\underline{2}$84 [25]		100	4	288 637884778574
	25	0	149.219456142191 [28]		150	6	541 591510339354
	30	0	217.287769647313		150	10	452.56677917451
	40	0	391.080887530226		200	0	1060.49730659884
	50	0	615.020090902757 [25]		200	10	790.294374761635
	100	0	2485 867880342075 [28]		250	20	899 697006946664
	100	38	1960.350416162349 [25]		350	30	1438 54384241202
	350	20	30070.3410019022		1000	100	6278 85555087975
8	200	0	518 386164077723	10	250	0	487 94744957
	300	0	906 804329278071		600	0	1520 075293620677
	400	2	1248 36413667149		750	2	1873.157090387933
	500	10	1308.16607088549		1000	4	2576 124759512495
	1000	12	3757 11868789022		2500	10	7958 935470023978
	5000	20	36818.2152343266		5000	20	18468 64455775824
	8000	50	64724.1278299979		12000	80	44168 83078468729
12	5000	2	15330.4550760349	14	6000	0	15583.5891495603
	10000	8	33956.5035261383		6000	4	14543.4675910831
	15000	10	55592.2396422714		10000	8	25750 0659173666
	15000	20	51929.9726421977		30000	2	101845.799152606
	20000	30	71149.4312776047		40000	2	142899 112064633
	2000	0	51858.1594416283		50000	4	184228 317084639
	4000	2	11644.3695556225		80000	10	314775.161831223
	80000	50	40116.8193850355		100000	20	399597.756264691
	100000	100	48594.4889916022		100000	50	368582.208502683

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